Modelling of High-Temperature Thermodynamic Properties of Metals

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Theoretical modelling, using a combination of molecular dynamics methods and ab initio electron structure calculations, has now reached an accuracy that allows a detailed analysis of the experimental heat capacity and other thermodynamic data of metals at high temperatures. Such an approach, when applied to, e.g., aluminum, leads to a reinterpretation of some experiments. For instance, what has previously been thought to be due to the thermal creation of divacancies is instead an effect of anharmonic effects in the properties of monovacancies. Furthermore, the heat capacity of Al at high temperatures and at constant volume is very close to the classical value for harmonic vibrations. This has previously been interpreted as a sign of an almost negligible anharmonicity at constant volume. The present analysis shows instead a cancellation at high temperatures between a significant low-order term that is linear in temperature, and higher-order anharmonic terms of opposite sign. Because molecular dynamics and ab initio electron structure calculations may replace costly experiments at high temperatures, it is important to assess their accuracy through a detailed analysis such as that presented here.